Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Methanol formation by catalytic hydrogenation of CO2 on nitrogen doped zinc oxide surface: An evaluative study on the mechanistic pathway by density functional theory

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The binding energies of CO_2 on $Zn_{18}O_{18}$ were calculated and shown in **Table 1.** The difference of -0.80 eV was observed between pure and nitrogen doped surface indicates the presence of N favors more adsorption than the pure state.

Table 1

	$Zn_{18}O_{17}$:N	**$Zn_{18}O_{18}$**
Binding energy	-1.86 eV	**-1.06 eV**

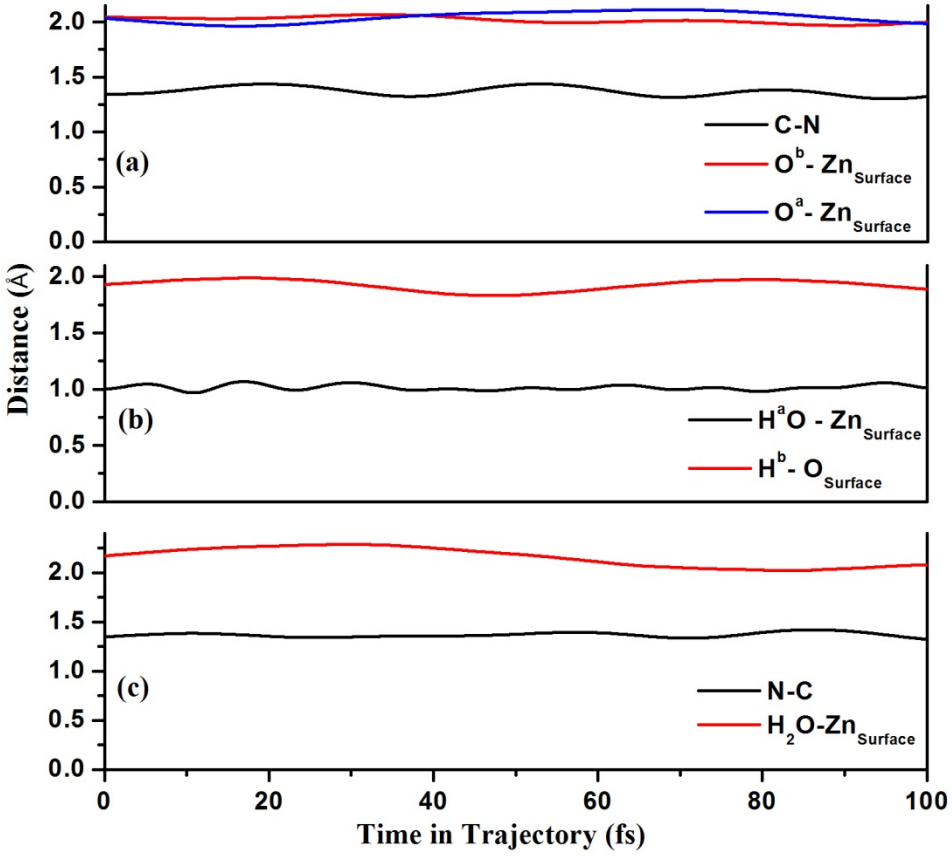

Figure 1. ADMP molecular dynamics profile of (a) carbamate, (b) dissociative adsorbed H_2O and (c) coadsorbed CO_2 & H_2O species on nitrogen doped zinc oxide clusters.